

# Self-Consistent Theory of Bose-Condensed Systems

V.I. Yukalov

*Bogolubov Laboratory of Theoretical Physics,  
Joint Institute for Nuclear Research, Dubna 141980, Russia  
and  
Theoretische Physik, Universität Essen,  
Universitätsstrasse 5, Essen 45117, Germany*

## Abstract

In the theory of Bose-condensed systems, there exists the well known problem, the Hohenberg-Martin dilemma of conserving versus gapless approximations. This dilemma is analysed and it is shown that it arises because of the internal inconsistency of the standard grand ensemble, as applied to Bose-systems with broken global gauge symmetry. A solution of the problem is proposed, based on the notion of representative statistical ensembles, taking into account all constraints imposed on the system. A general approach for constructing representative ensembles is formulated. Applying a representative ensemble to Bose-condensed systems results in a completely self-consistent theory, both conserving and gapless in any approximation.

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## 1 Introduction

Bose-Einstein condensation in Bose systems is commonly associated with the global gauge symmetry breaking. The most general way of the gauge symmetry breaking is by means of the Bogolubov shift in the field operators [1–4]. In his first works [1,2], Bogolubov considered a weakly-nonideal Bose gas in the limit of a small condensate depletion, which can occur at low temperatures and asymptotically weak interactions. The following generalization of the Bogolubov ideas, based on the standard grand ensemble with broken gauge symmetry, confronted the well known problem of theories being either nonconserving or exhibiting an unphysical gap in the spectrum. Hohenberg and Martin [5] were, probably, the first who analysed in detail this dilemma and classified the approaches onto conserving versus gapless. In a nonconserving theory, the dynamic conservation laws are not valid and general thermodynamic relations do not hold, which is related to the thermodynamic instability of the system. If the theory is conserving, but exhibits a gap in the spectrum, it also has incorrect thermodynamics and contradicts the theorems of the gapless spectrum by Bogolubov [4] and Hugenholtz and Pines [6]. A thorough discussion of the Hohenberg-Martin dilemma has recently been done by Andersen [7], where the extensive literature on the problem is cited.

It is important to emphasize that the inconsistency, happening in the theory, is internal, but not connected with the employed approximations. Really, suppose one applies the standard grand ensemble, with a chemical potential  $\mu$ , to an equilibrium Bose-condensed system. After breaking the gauge symmetry, by means of the Bogolubov shift, one has to minimize the grand thermodynamic potential with respect to the number of condensed particles  $N_0$ . Bogolubov [1–4] illustrated this procedure for a weakly nonideal gas. Ginibre [8] proved that this procedure is general for arbitrary Bose systems. The Bogolubov-Ginibre minimization procedure defines the chemical potential  $\mu \rightarrow \mu_{BG}(\rho, T)$  as a function of density  $\rho$  and temperature  $T$ .

On the other hand, there exists the Hugenholtz-Pines relation [6] also defining the chemical potential  $\mu \rightarrow \mu_{HP}(\rho, T)$ . The most general proof on this relation, for any Bose system and arbitrary temperatures, is based on the consideration of increments of statistical averages under gauge variations [4]. This is analogous to the consideration of the Ward-Takahashi identity. The Hugenholtz-Pines relation follows from the symmetry of the Hamiltonian, but is not connected with the system stability.

Thus, there are two representations for the chemical potential. One,  $\mu_{BG}$ , is a consequence of the condition of thermodynamic stability, while another,  $\mu_{HP}$ , results from the symmetry properties. Two different, both physically and mathematically, conditions do not need to define one and the same quantity, so that generally,  $\mu_{BG} \neq \mu_{HP}$ . And this is exactly what happens [5,7], making the theory not self-consistent.

So, it is not some particular approximations that are guilty for the arising inconsistency. Also, the gauge symmetry breaking is not to be blamed. The concept of symmetry breaking under phase transitions is rather general [9,10]. But the inconsistency, related to the inequality  $\mu_{BG} \neq \mu_{HP}$ , is generic for the used statistical ensemble.

The Hohenberg-Martin dilemma has been addressed in a number of papers. One usually attempts to cure the problem in a mean-field approximation complemented by some phenomenological tricks. The most common, and the least justified, trick is by omitting the anomalous averages. One often ascribes this trick to Popov, terming it the "Popov approximation". First of all, however, it is not difficult to infer from the original works by Popov [11–13], cited in this regard, that he has never suggested or used such an unjustified trick. The person who really first proposed and employed the trick was Shohno [14]. This was known in literature as Shohno model. But in the case of the broken gauge symmetry the anomalous averages become principally important and cannot be omitted. Direct calculations [15] show that the anomalous averages at low temperatures can be even much larger than the normal ones. So, neglecting the terms that are larger than what is left cannot be a reasonable mathematical approximation. In addition, the omission of anomalous averages renders the system thermodynamically unstable [15,16], with incorrect thermodynamics [17].

To remove the gap in the spectrum, one sometimes resorts to what Bogolubov [4] called the mismatch of approximations. Then one defines the chemical potential  $\mu_{BG}$  from the condition of thermodynamic stability in one approximation, but, for cancelling the appearing gap, one invokes the self-energies in another, higher, approximation, or just adding phenomenological terms. As is evident, the mismatch of approximations is not a logical procedure, is not uniquely defined, and does not solve the problem that for each given approximation the theory remains not self-consistent. Also, the mismatch

of approximations leads to incorrect thermodynamics, with a first-order phase transition, instead of the second-order one [18–20]. Thermodynamic self-consistency can be preserved only when all quantities are derived from the same Hamiltonian in the same chosen approximation [21,22].

As is mentioned above, the inconsistency, manifesting itself in the inequality  $\mu_{BG} \neq \mu_{HP}$ , is generic for the used statistical ensemble and does not depend on the employed approximations. The problem can be solved by using a representative statistical ensemble, which takes into account all constraints imposed on the Bose-condensed system [23]. Then, for instance, the Hartree-Fock-Bogolubov (HFB) approximation can be made conserving and gapless [24].

In the present paper, the general notion of representative statistical ensembles is formulated for arbitrary statistical systems. The representative ensemble for a Bose-condensed system is defined. It is shown that the theory, based on the representative ensemble, is completely self-consistent, independently of the used approximations. This solves the Hohenberg-Martin dilemma, suggesting an approach that is free from inconsistencies and paradoxes.

Everywhere, below the system of units is used, where  $\hbar \equiv 1$  and  $k_B \equiv 1$ .

## 2 Representative Ensembles

It was already Gibbs [25] himself who mentioned that for a correct description of a statistical system, in addition to a canonical distribution, one has to accurately take into account all conditions and constraints, imposed on the system and uniquely representing its properties. From this general idea stems the term "representative ensembles", which was used by ter Haar [26,27]. For equilibrium systems, one defines representative ensembles through the conditional maximization of the Gibbs entropy, as was done by Janes [28]. A generalization for quasi-equilibrium systems was given in Ref. [29]. Here, we describe a general method for constructing representative ensembles for both equilibrium and nonequilibrium systems.

An *equilibrium statistical ensemble* is a pair  $\{\mathcal{F}, \hat{\rho}\}$  of a space of microstates  $\mathcal{F}$  and a statistical operator  $\hat{\rho}$  on this space. Let a set  $\{\hat{C}_i\}$  of self-adjoint operators  $\hat{C}_i$  be given, which we shall call the condition operators, since these define the *statistical conditions*

$$C_i = \langle \hat{C}_i \rangle = \text{Tr} \hat{\rho} \hat{C}_i, \quad (1)$$

which are assumed to be imposed on the considered system. The trace operation in Eq. (1) is over the space of microstates  $\mathcal{F}$ . One obvious constraint is the normalization condition for the statistical operator,

$$1 = \langle \hat{1}_{\mathcal{F}} \rangle = \text{Tr} \hat{\rho}, \quad (2)$$

where  $\hat{1}_{\mathcal{F}}$  is the unity operator in  $\mathcal{F}$ . Another standard condition is the definition of the internal energy

$$E = \langle \hat{H} \rangle = \text{Tr} \hat{\rho} \hat{H} \quad (3)$$

as the average of a Hamiltonian  $\hat{H}$ . However, in addition to these standard conditions, other statistical conditions (1) can also be necessary for correctly representing the system.

For the conditional maximization of the Gibbs entropy  $S \equiv -\text{Tr} \hat{\rho} \ln \hat{\rho}$ , under statistical conditions (1), (2), and (3), it is convenient to introduce [30] the *information functional*

$$I[\hat{\rho}] = \text{Tr} \hat{\rho} \ln \hat{\rho} + \lambda_0 (\text{Tr} \hat{\rho} - 1) + \beta (\text{Tr} \hat{\rho} \hat{H} - E) + \beta \sum_i \nu_i (\text{Tr} \hat{\rho} \hat{C}_i - C_i) , \quad (4)$$

with the Lagrange multipliers  $\lambda_0$ ,  $\beta$ , and  $\beta \nu_i$ . The statistical operator is given by the minimum of the information functional (4),

$$\hat{\rho} = \frac{1}{Z} e^{-\beta H} , \quad (5)$$

with the *grand Hamiltonian*

$$H \equiv \hat{H} + \sum_i \nu_i \hat{C}_i . \quad (6)$$

Here  $Z \equiv \exp(1 + \lambda_0)$  is the partition function and  $\beta \equiv T^{-1}$  is inverse temperature.

The *representative statistical ensemble* for an equilibrium system under constraints (1), (2), and (3), is the pair  $\{\mathcal{F}, \hat{\rho}\}$  of a space of microstates  $\mathcal{F}$  and the statistical operator (5) with the grand Hamiltonian (6).

Note that the condition operators  $\hat{C}_i$  are to be self-adjoint, but they do not need to be compulsorily the integrals of motion. Thus, the number-of-particle operator  $\hat{N}$  is not an integral of motion, when the gauge symmetry is broken.

A *nonequilibrium statistical ensemble* is a triplet  $\{\mathcal{F}, \hat{\rho}, \partial/\partial t\}$  of a space of microstates  $\mathcal{F}$ , the statistical operator  $\hat{\rho} \equiv \hat{\rho}(0)$  at the initial time  $t = 0$ , and of a prescribed evolution law, symbolically denoted here as  $\partial/\partial t$ . The law of evolution can be given as the Liouville equation for the time-dependent statistical operator  $\hat{\rho}(t)$  or as the Heisenberg equations of motion for physical operators, or in some other form. A general way of deriving the evolution equations is by extremizing an effective action functional with respect to the given dynamical variables [31].

To construct an action functional, one defines the corresponding Lagrangian

$$\hat{L} \equiv \hat{E} - \hat{H} , \quad (7)$$

in which  $\hat{E}$  is the time-dependent energy operator, containing the time derivative. The effective action, for a system with the Lagrangian (7), under constraints (1), is

$$A = \int (\hat{L} - \nu_i \hat{C}_i) dt , \quad (8)$$

where  $\nu_i$  are the Lagrange multipliers. Equation (8) can be rewritten as

$$A = \int (\hat{E} - H) dt , \quad (9)$$

with the same grand Hamiltonian (6). The evolution equations follow from the extremization of the effective action,  $\delta A = 0$ . For instance, if the effective action  $A = A[\psi]$  is a functional of field operators  $\psi(\mathbf{r}, t)$  and  $\psi^\dagger(\mathbf{r}, t)$ , then the latter satisfy the equations

$$\frac{\delta A[\psi]}{\delta \psi^\dagger(\mathbf{r}, t)} = 0 , \quad \frac{\delta A[\psi]}{\delta \psi(\mathbf{r}, t)} = 0 . \quad (10)$$

The grand Hamiltonian (6) governs both the statistical properties of equilibrium systems and the temporal evolution of nonequilibrium systems.

### 3 Bose Systems

Let us consider a one-component system of spinless particles characterized by the field operators  $\psi$  and  $\psi^\dagger$  satisfying the Bose commutation relations. For the system above the critical temperature  $T_c$ , the space of microstates is the Fock space  $\mathcal{F}(\psi)$  generated by the field operators [30–32]. In addition to statistical conditions (2) and (3), there is one normalization condition for the total number of particles  $N = \langle \hat{N} \rangle$ . Hence, the grand Hamiltonian (6) is  $H = \hat{H} - \mu \hat{N}$ , where  $\mu$  is the usual chemical potential.

However, the situation changes below the critical temperature  $T_c$ , when the global gauge symmetry becomes broken. The symmetry breaking is realized by the Bogolubov shift

$$\psi(\mathbf{r}, t) \longrightarrow \hat{\psi}(\mathbf{r}, t) \equiv \eta(\mathbf{r}, t) + \psi_1(\mathbf{r}, t) , \quad (11)$$

in which  $\eta(\mathbf{r}, t)$  is the condensate wave function and  $\psi_1(\mathbf{r}, t)$  is the field operator of uncondensed particles. The field operators  $\psi_1$  and  $\psi_1^\dagger$  generate the Fock space  $\mathcal{F}(\psi_1)$ , which is the space of microstates for the system with broken gauge symmetry. The spaces of microstates  $\mathcal{F}(\psi)$ , for the system above  $T_c$ , and  $\mathcal{F}(\psi_1)$ , for the system below  $T_c$ , are mutually orthogonal [33,34].

For the system with broken gauge symmetry, there are now two variables, the condensate wave function  $\eta$  and the field operator of uncondensed particles  $\psi_1$ . These variables are assumed to be linearly independent, being orthogonal to each other,

$$\int \eta^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) d\mathbf{r} = 0 . \quad (12)$$

Respectively, instead of one normalization condition for the total number of particles, we have now two normalization conditions, for the number of condensed particles

$$N_0 = \langle \hat{N}_0 \rangle , \quad (13)$$

where, the average is over the space  $\mathcal{F}(\psi_1)$ ,  $\hat{N}_0 \equiv N_0 \hat{1}_{\mathcal{F}}$ ,  $\hat{1}_{\mathcal{F}}$  being a unity operator in  $\mathcal{F}(\psi_1)$ , and

$$N_0 = \int |\eta(\mathbf{r}, t)|^2 d\mathbf{r} , \quad (14)$$

and for the number of uncondensed particles

$$N_1 = \langle \hat{N}_1 \rangle , \quad (15)$$

with the operator of uncondensed particles

$$\hat{N}_1 \equiv \int \psi_1^\dagger(\mathbf{r}, t) \psi_1(\mathbf{r}, t) d\mathbf{r} . \quad (16)$$

The total number of particles is  $N = N_0 + N_1$ .

With the broken gauge symmetry, the average  $\langle \psi_1 \rangle$  might be nonzero. This, however, would mean that quantum numbers, such as spin or momentum, would not be conserved. To avoid this, one implies the constraint

$$\langle \psi_1(\mathbf{r}, t) \rangle = 0 , \quad (17)$$

guaranteeing the conservation of quantum numbers. Constraint (17) can be represented in the standard form (1) of a statistical condition by introducing the self-adjoint operator

$$\hat{\Lambda} \equiv \int \left[ \lambda(\mathbf{r}, t) \psi_1^\dagger(\mathbf{r}, t) + \lambda^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \right] d\mathbf{r} , \quad (18)$$

in which  $\lambda(\mathbf{r}, t)$  is a complex function. Then constraint (17) is equivalent to the *quantum conservation condition*

$$\langle \hat{\Lambda} \rangle = 0 . \quad (19)$$

Thus, for a system with broken gauge symmetry, there are three statistical conditions, (13), (15) and (19). To construct the corresponding representative ensemble, we have to follow the general prescription of Sec. 2.

For a system in equilibrium, in view of Eq. (4), the information functional is

$$\begin{aligned} I[\hat{\rho}] = & \text{Tr} \hat{\rho} \ln \hat{\rho} + \lambda_0 (\text{Tr} \hat{\rho} - 1) + \beta (\text{Tr} \hat{\rho} \hat{H} - E) - \\ & - \beta \mu_0 (\text{Tr} \hat{\rho} \hat{N}_0 - N_0) - \beta \mu_1 (\text{Tr} \hat{\rho} \hat{N}_1 - N_1) - \beta \text{Tr} \hat{\rho} \hat{\Lambda} . \end{aligned} \quad (20)$$

The minimization of this functional yields the statistical operator (5) with the grand Hamiltonian

$$H = \hat{H} - \mu_0 \hat{N}_0 - \mu_1 \hat{N}_1 - \hat{\Lambda} , \quad (21)$$

in agreement with Eq. (6).

In the general case of a nonequilibrium system, we need to consider the Lagrangian (7), in which the temporal energy operator is

$$\hat{E} = \int \left[ \eta^*(\mathbf{r}, t) i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) + \psi_1^\dagger(\mathbf{r}, t) i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) \right] d\mathbf{r} .$$

The action functional (9) has to be extremized with respect to two linearly independent variables,  $\eta$  and  $\psi_1$ , which implies

$$\frac{\delta A[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)} = 0 , \quad \frac{\delta A[\eta, \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} = 0 . \quad (22)$$

The latter is equivalent to the equations

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)} , \quad i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} . \quad (23)$$

The average of the grand Hamiltonian (21) is

$$\langle H \rangle = E - \mu_0 N_0 - \mu_1 N_1 . \quad (24)$$

If in experiment only the total number of particles, or the total average density, can be fixed, then average (24) should be expressed in the standard form  $\langle H \rangle = E - \mu N$  through the system chemical potential  $\mu$ . Comparing this with Eq. (24) defines the chemical potential

$$\mu = \mu_0 n_0 + \mu_1 n_1 \quad (25)$$

through the Lagrange multipliers  $\mu_0$  and  $\mu_1$  and through the fractions  $n_0 \equiv N_0/N$  and  $n_1 \equiv N_1/N$ .

Let us take the Hamiltonian energy operator in the usual form

$$\begin{aligned} \hat{H} = & \int \hat{\psi}^\dagger(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U \right) \hat{\psi}(\mathbf{r}) d\mathbf{r} + \\ & + \frac{1}{2} \int \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) d\mathbf{r} d\mathbf{r}', \end{aligned} \quad (26)$$

in which  $\hat{\psi}(\mathbf{r}) = \hat{\psi}(\mathbf{r}, t)$  is the Bogolubov shifted field operator  $\hat{\psi} \equiv \eta + \psi_1$ , defined in Eq. (11). Here  $U = U(\mathbf{r}, t)$  is an external potential. The interaction potential  $\Phi(\mathbf{r})$  is symmetric, so that  $\Phi(-\mathbf{r}) = \Phi(\mathbf{r})$ , and is assumed to possess the Fourier transform. With the Bogolubov shift (11), Hamiltonian (26) can be represented as a sum of five terms,  $H = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} + H^{(4)}$ , depending on the powers of the operators  $\psi_1$  and  $\psi_1^\dagger$  in each of them [34]. The zero-order term  $H^{(0)}$  contains no  $\psi_1$ . The necessary and sufficient condition for the validity of constraint (19) is the absence in the Hamiltonian of terms linear in  $\psi_1$  [35]. This requires to define the Lagrange multipliers  $\lambda(\mathbf{r}, t)$  such that  $H^{(1)} = 0$ .

The evolution equations (23) give

$$\begin{aligned} i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = & \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}, t) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ |\eta(\mathbf{r}')|^2 \eta(\mathbf{r}) + \hat{X}(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}', \\ i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = & \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}, t) + \\ & + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ |\eta(\mathbf{r}')|^2 \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \eta(\mathbf{r}) \psi_1(\mathbf{r}') + \eta(\mathbf{r}') \eta(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') + \hat{X}(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}', \end{aligned} \quad (27)$$

where, for brevity, the time dependence in the integrands is not shown explicitly and the notation for the correlation operator

$$\begin{aligned} \hat{X}(\mathbf{r}, \mathbf{r}') \equiv & \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \eta(\mathbf{r}) + \\ & + \psi_1^\dagger(\mathbf{r}') \eta(\mathbf{r}') \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \end{aligned}$$

is used. It is straightforward to check that the evolution equations (27) guarantee the validity of all local conservation laws on the operator level, as it should be for the equations derived from a variational procedure.

Averaging the first of Eqs. (27) over  $\mathcal{F}(\psi_1)$ , we obtain the explicit equation for the condensate wave function

$$\begin{aligned} i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = & \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}, t) + \\ & + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \xi(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}', \end{aligned} \quad (28)$$

in which

$$\rho_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}) \rangle, \quad \sigma_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle,$$

$$\xi(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle ,$$

$$\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) , \quad \rho_0(\mathbf{r}) \equiv |\eta(\mathbf{r})|^2 , \quad \rho_1(\mathbf{r}) \equiv \rho_1(\mathbf{r}, \mathbf{r}) = \langle \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) \rangle .$$

Equation (28) is valid for an arbitrary Bose system. For a system in equilibrium, we require that the condensate function be time independent,  $\partial\eta/\partial t = 0$ . If, in addition, the system is uniform, with no external fields, then Eq. (28) yields

$$\mu_0 = \rho\Phi_0 + \int \Phi(\mathbf{r}) \left[ \rho_1(\mathbf{r}, 0) + \sigma_1(\mathbf{r}, 0) + \frac{\xi(\mathbf{r}, 0)}{\sqrt{\rho_0}} \right] d\mathbf{r} . \quad (29)$$

The matrix Green function  $G(12)$  for uncondensed particles is defined in the usual way [4–6], where the common abbreviation can be employed, denoting the set  $\{\mathbf{r}_j, t_j\}$  by a single number  $j$ . The elements of this matrix are

$$G_{11}(12) = -i \langle \hat{T} \psi_1(1) \psi_1^\dagger(2) \rangle , \quad G_{12}(12) = -i \langle \hat{T} \psi_1(1) \psi_1(2) \rangle ,$$

$$G_{21}(12) = -i \langle \hat{T} \psi_1^\dagger(1) \psi_1^\dagger(2) \rangle , \quad G_{22}(12) = -i \langle \hat{T} \psi_1^\dagger(1) \psi_1(2) \rangle , \quad (30)$$

where  $\hat{T}$  is the chronological operator. For an equilibrium system, we may pass to the Fourier transform  $G(\mathbf{k}, \omega)$  of  $G(12)$ . Equations of motion give

$$G_{11}(\mathbf{k}, \omega) = \frac{\omega + k^2/2m + \Sigma_{11}(\mathbf{k}, \omega) - \mu_1}{D(\mathbf{k}, \omega)} ,$$

$$G_{12}(\mathbf{k}, \omega) = - \frac{\Sigma_{12}(\mathbf{k}, \omega)}{D(\mathbf{k}, \omega)} = G_{21}(\mathbf{k}, \omega) , \quad (31)$$

where  $\Sigma(\mathbf{k}, \omega) = [\Sigma_{\alpha\beta}(\mathbf{k}, \omega)]$  is the self-energy matrix, and the denominator is given by the equations

$$D(\mathbf{k}, \omega) \equiv \Sigma_{12}^2(\mathbf{k}, \omega) - G_{11}^{-1}(\mathbf{k}, \omega) G_{11}^{-1}(\mathbf{k}, -\omega) ,$$

$$G_{11}^{-1}(\mathbf{k}, \omega) = \omega - \frac{k^2}{2m} - \Sigma_{11}(\mathbf{k}, \omega) + \mu_1 .$$

From the Bogolubov theorem [4], we have

$$|G_{11}(\mathbf{k}, 0) - G_{12}(\mathbf{k}, 0)| \geq \frac{mn_0}{k^2} . \quad (32)$$

Using here Eqs. (31), we obtain the Hugenholtz-Pines relation

$$\mu_1 = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0) , \quad (33)$$

which makes the spectrum gapless.

Comparing Eqs. (29) and (33), we see that these expressions are rather different, and there is no reason to require that  $\mu_0$  be equal to  $\mu_1$ . As an illustration, we can resort to the Hartree-Fock-Bogolubov (HFB) approximation, in which we find

$$\mu_0 = \rho\Phi_0 + \frac{1}{V} \sum_{p \neq 0} (n_p + \sigma_p) \Phi_p , \quad \mu_1 = \rho\Phi_0 + \frac{1}{V} \sum_{p \neq 0} (n_p - \sigma_p) \Phi_p , \quad (34)$$



where  $V$  is the system volume,  $\Phi_p$  is the Fourier transform of  $\Phi(\mathbf{r})$  and  $n_p$  and  $\sigma_p$  are the normal and anomalous averages, respectively, in the momentum space,

$$n_k \equiv \langle a_k^\dagger a_k \rangle , \quad \sigma_k \equiv \langle a_k a_{-k} \rangle ,$$

with  $a_k$  being the Fourier transform of  $\psi_1(\mathbf{r})$ . Clearly,  $\mu_0 \neq \mu_1$ . The anomalous average  $\sigma_k$ , as can be shown by direct calculations [15,24], can be much larger than the normal average  $n_k$ . Hence, there is no any sense in omitting  $\sigma_k$ . As has also been mentioned above, the presence of  $\sigma_k$  is crucially important for the stability of the system [15,16,23,36].

The physics of dilute Bose gases has resently attracted a great deal of attention, both experimentally and theoretically (see review works [7,37–40]). These gases are described by the local interaction potential

$$\Phi(\mathbf{r}) = \Phi_0 \delta(\mathbf{r}) , \quad \Phi_0 \equiv 4\pi \frac{a_s}{m} , \quad (35)$$

in which  $a_s$  is the scattering length. For this potential, Eqs. (34) reduce to

$$\mu_0 = (\rho + \rho_1 + \sigma_1)\Phi_0 , \quad \mu_1 = (\rho + \rho_1 - \sigma_1)\Phi_0 , \quad (36)$$

where

$$\rho_1 = \frac{1}{V} \sum_{k \neq 0} n_k , \quad \sigma_1 = \frac{1}{V} \sum_{k \neq 0} \sigma_k .$$

The particle spectrum has the Bogolubov form

$$\varepsilon_k = \sqrt{(ck)^2 + \left(\frac{k^2}{2m}\right)^2} ,$$

with the sound velocity  $c$  defined by the equation

$$mc^2 = (\rho_0 + \sigma_1)\Phi_0 , \quad (37)$$

where  $\rho_0 \equiv N_0/V$  is the condensate density. The anomalous average  $\sigma_1$ , invoking the dimensional regularization, can be represented as

$$\sigma_1 = \frac{(mc)^2}{\pi^2} \sqrt{m\rho_0\Phi_0} - \frac{(mc)^3}{2\sqrt{2}\pi} \int_0^\infty \frac{(\sqrt{1+x^2}-1)^{1/2}}{\sqrt{1+x^2}} \left[ \coth\left(\frac{mc^2}{2T}\right) - 1 \right] dx . \quad (38)$$

The condensate fraction becomes

$$n_0 = 1 - \frac{(mc)^3}{3\pi^2\rho} \left\{ 1 + \frac{3}{2\sqrt{2}} \int_0^\infty (\sqrt{1+x^2}-1)^{1/2} \left[ \coth\left(\frac{mc^2}{2T} x\right) - 1 \right] dx \right\} . \quad (39)$$

And for the superfluid fraction, defined through the response to a velocity boost [37], we obtain

$$n_s = 1 - \frac{(mc)^3 mc^2}{6\sqrt{2}\pi^2\rho T} \int_0^\infty \frac{(\sqrt{1+x^2}-1)^{3/2} x dx}{\sqrt{1+x^2} \sinh^2(mc^2 x/2T)} . \quad (40)$$

The above equations show that the system undergoes the second-order phase transition at the critical temperature

$$T_c = \frac{2\pi}{m} \left[ \frac{\rho}{\zeta(3/2)} \right]^{2/3}$$

coinciding with that for the ideal gas, as it should be for a mean-field approximation with the local interaction potential (35). Note that all integrals in Eqs. (38), (39), and (40) are well defined and convergent.

In conclusion, the old-standing problem, the Hohenberg-Martin dilemma, is analysed, which classifies the theories of Bose-condensed systems onto either conserving or gapless. This dilemma is shown to be of general nature, not dependent on the used approximations, and having its footing in the generic inconsistency of the standard grand ensemble applied to the Bose systems with broken global gauge symmetry. The notion of representative statistical ensembles for arbitrary systems is formulated. A representative ensemble uniquely represents the given statistical system by taking into account all constraints and conditions imposed on the system. The usage of representative ensembles for Bose-condensed system provides the remedy from internal inconsistencies, cures old paradoxes, and gives the solution to the Hohenberg-Martin dilemma. The suggested theory for Bose-condensed systems, based on a representative ensemble, is completely self-consistent, conserving, and gapless. This is achieved by introducing two Lagrange multipliers,  $\mu_0$  and  $\mu_1$ , which are responsible for two normalization conditions, for  $N_0$  and  $N_1$ , respectively. Note that in the current experiments with trapped atoms [37–40] two atomic numbers can be controlled, the total number of atoms  $N$  and the number of condensed atoms  $N_0$ . In addition, the operator  $\hat{N}_0$  is the integral of motion, since  $[\hat{N}_0, H] = 0$ . So, fixing two normalization conditions is justified both mathematically as well as physically. Two Lagrange multipliers are necessary in order to uniquely define the condensate wave function, which is a two-component order parameter. This agrees with the general rule for any statistical system:

*To uniquely define an order parameter of a system, it is necessary to introduce as many Lagrange multipliers as is the number of components in the order parameter.*

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